OMS

Organic Mass Spectrometry

1994 **Volume 29**

ORMSBG 29(1–12) 1–812 (1994)
ISSN 0030–493X

WILEY
Publishers Since 1807

Organic Mass Spectrometry

(*Org. mass spectrom.*)

EDITORS

Professor B. T. CHAIT

The Rockefeller University, 1230 York Avenue, New York, NY 10021-6399, USA
Specialist office: Ion formation from biological solids

Professor O. S. CHIZHOV

N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Leninsky Prospect 47, Moscow 117334, Russia

Professor H.-Fr. GRÜTZMACHER

Fakultät für Chemie, Universität Bielefeld, PO Box 8640, 48 Bielefeld, Universitätsstrasse 25, Germany.

Dr J. K. MACLEOD

Research School of Chemistry, Australian National University, Canberra, A.C.T. 2600, Australia

Professor M. ÔHASHI

Department of Applied Physics and Chemistry, The University of Electro-Communication, Chofu, Tokyo 182, Japan

Professor D. P. RIDGE

Department of Chemistry, University of Delaware, Newark, Delaware 19711, USA
Specialist office: Ion–molecule reactions

Professor F. TURECEK

Department of Chemistry, BG-10, University of Washington, Seattle, Washington 98195, USA

EX OFFICIO MEMBERS

J. H. Beynon, FRS
Editor-in-Chief, *Rapid Communications in Mass Spectrometry*

R. M. Caprioli
Editor-in-Chief, *Biological Mass Spectrometry*

ADVISORY BOARD

Prof. T. Ast, *University of Belgrade*
Prof. A. Benninghoven, *University of Munster*
Prof. H. Budzikiewicz, *University of Cologne*
Prof. M. M. Bursey, *University of North Carolina*
Prof. R. G. Cooks, *Purdue University*
Dr C. Costello, *Massachusetts Institute of Technology*
Dr F. H. Cottee, *SmithKline Beecham Pharmaceuticals*
Prof. F. De Angelis, *University of l'Aquila*
Dr S. Della Negra, *Institut de Physique Nucleaire, Orsay*
Prof. M. L. Gross, *Washington University*
Prof. J. Grotemeyer, *University of Wurzburg*
Dr S. Hammerum, *University of Copenhagen*
Dr V. Hanus, *Czechoslovak Academy of Science, Prague*
Prof. A. G. Harrison, *University of Toronto*
Prof. J. L. Holmes, *University of Ottawa*
Dr Y. Hoppilliard, *Ecole Polytechnique*
Prof. K. R. Jennings, *Warwick University*
Prof. F. W. McLafferty, *Cornell University*
Prof. A. Mandelbaum, *Technion, Haifa*
Prof. T. Matsuo, *Osaka University*
Prof. N. M. M. Nibbering, *University of Amsterdam*
Prof. F. W. Röllgen, *University of Bonn*
Dr B. Rozynov, *Russian Academy of Sciences*
Prof. D. H. Russell, *Texas A & M University*
Prof. A. Selva, *Milan Polytechnic*
Prof. B. U. R. Sundqvist, *Uppsala University*
Prof. A. Tatematsu, *Meijo University*
Prof. J. K. Terlouw, *McMaster University*
Prof. J. F. J. Todd, *University of Kent, Canterbury*
Prof. M. Tsuchiya, *Yokohama National University*
Prof. V. G. Zaikin, *Russian Academy of Sciences*

Copyright © 1994 by John Wiley & Sons, Ltd.

COPYING OF ARTICLES

The code and the copyright notice appearing at the bottom of the first page of an article in this journal indicates the copyright owner's consent that copies of the article may be made for personal or internal use, or for the personal or internal use of specific clients, on the condition that the copier pay for copying beyond that permitted by Sections 107 or 108 of the US Copyright Law. The per-copy fee for each article appears after the dollar sign, and is to be paid through the Copyright Clearance Center Inc. This consent does not extend to other kinds of copying, such as copying for general distribution, for advertising or promotional purposes, for creating new collective works, or for resale. Such permission requests, or other inquiries, should be addressed to the publisher.

Printed in Great Britain by Page Bros (Norwich) Ltd, Norwich

Contents of Volume 29

NUMBER 1 JANUARY 1994

Long-lived Distonic Radical Cations 1
H. I. KENTTÄMAA

Neutral Counterparts of the $C_2H_7O^+$ Isomers 11
M. SIROIS, M. GEORGE AND J. L. HOLMES

Systematic Study of the Effects of Experimental Parameters on the Beam-induced Dehalogenation of Chlorpromazine in Liquid Secondary Ion Mass Spectrometry 18
R. THÉBERGE, G. J. C. PAUL AND M. J. BERTRAND

The *Ortho* Effect in the Mass Spectra of *Ortho*/*Para* Isomers of Bisphenol A Derivatives and Related Compounds 26
A. P. PLESHKOVA, M. N. USPENSKAYA AND S. V. VOLKOVITCH

Photodissociation and Collision-induced Dissociation of Molecular Ions from Methylphenol and Chloromethylphenol 30
C. J. CASSADY, S. AFZAAL AND B. S. FREISER

Mass Spectrometry of Some 10β-Fluoro-1,4-estradien-3-oxo Steroids 37
D. D. DESMARTEAU, G. RESNATI, R. SERAGLIA AND P. TRALDI

Influence of Fluorine Atoms on the Electron Impact and Chemical Ionization Mass Spectrometric Fragmentation of Methyl *x*-Deoxy-*x*-fluoro-per-*O*-methyl-β-D-galactopyranosides 44
V. KOVÁČIK AND P. KOVÁČ

Alkylation in Electron Impact Mass Spectrometry of Hydrobromides of 2-Alkylthioorotic Acids 50
E. WYRZYKIEWICZ AND G. BARTKOWIAK

OMS Letters

The Proton Affinity of Methyl Nitrate 55
A. RICCI

Gas-phase Ion Chemistry of Carbon Suboxide 57
L. PANDOLFO, G. PAIARO, S. CATINELLA, P. TRALDI AND P. DERRICK

Diary 60

NUMBER 2 FEBRUARY 1994

Mass Spectrometry, Carbon Clusters and Coal 61
P. F. GREENWOOD

Investigation of the Effects of Cooling After Laser Desorption Before Post-ionization 78
R. J. J. M. STEENVOORDEN, E. R. E. VAN DER HAGE, J. J. BOON, P. G. KISTEMAKER AND T. L. WEEDING

Fingerprinting Stereoisomers by Survivor-ion Mass Spectrometry 85
M. GU AND F. TURECEK

Unimolecular Reactions of $^{\cdot}CH_2CH_2\overset{+}{O}HCH_2CH_2CH_3$ β-Distonic Ion 90
A. MILLIET, E. LECARPENTIER AND H.-E. AUDIER

Ion Cyclotron Resonance Mass Spectrometry Study of Ion-molecule Reactions in Toluene-pyridine Mixtures 96
A. R. KATRITSKY, Z. DEGA-SZAFRAN, R. RAMANATHAN AND J. R. EYLER

Mass Spectrometric Study on 2–Acyloxy-4,6-dimethoxy–1,3,5–triazines 102
M. SOCHACKI AND Z. J. KAMIŃSKI

Heat of Formation of the Radical Cation of Dimethyl Disulfide 106
D. T. LEECK AND H. I. KENTTÄMAA

Rapid Molecular Mass Determination of Mono–, Di– and Triglycerides by ^{252}Cf Plasma Desorption Mass Spectrometry Using 3–(3–Pyridyl)acrylic Acid as Matrix 108
E. PITTENAUER, G. ALLMAIER AND E. R. SCHMID

Diary 112

NUMBER 3 MARCH 1994

Mass Spectrometric Fragmentation of Isomeric 2–Alkyl–substituted 1,3–Indandiones and 3–Alkylidenephthalides: A Seven-step Consecutive Isomerization of Regular and Distonic Molecular Radical Cations 113
D. KUCK

Electron and Chemical Ionization Mass Spectrometry in Stereochemical Differentiation of Some 1,3–Amino Alcohols 126
T. PARTANEN, P. VAINIOTALO, G. STÁJER, G. BERNÁTH AND K. PIHLAJA

Dechlorination of Polychlorinated Biphenyls in Electron–capture Negative-ion Chemical Ionization Mass Spectrometry 133
F. L. LÉPINE, S. M. MILOT, M. L. J. REIMER AND O. A. MAMER

Collision-induced Decompositions of Metal-cationized Methyl–6–deoxy–6–Bromo–α–D–glucopyranoside Derivatives 143
K. P. MADHUSUDANAN, T. S. DHAMI, S. KATIYAR AND S. N. SURYAWANSHI

OMS Letters

How Does Isotopic Substitution Effect the Gas-phase Proton Affinity of Glycine? A Combined Experimental and *Ab Initio* Study 151
R. A. O'HAIR, S. GRONERT AND T. D. WILLIAMS

Propene Loss from Phenylpropylmethyleneiminium Ions 153
J. H. GROSS AND H. J. VEITH

Generation and Metastable Ion Characterization of the Pair of Radical Cation Keto/Enol Tautomers of Phenylketene 155
A. A. A. SHOKHBA, H. YAMAOKA, K. HORI, R. H. FOKKENS AND N. M. M. NIBBERING

Diary 157

NUMBER 4 APRIL 1994

Collision-induced Dissociation Studies of Protonated Alcohol and Alcohol-Water Clusters by Atmospheric Pressure Ionization Tandem Mass Spectrometry. 1—Methanol 159
Z. KARPAS, G. A. EICEMAN, C. S. HARDEN, R. G. EWING AND P. B. W. SMITH

Matrix Influence on Stability Constants of 15-Crown-5–Alkali Metal Complexes Measured by Liquid Secondary Ion Mass Spectrometry 169
D. GIRAUD, O. LAPRÉVOTE AND B. C. DAS

Methoxymethyl Cation $[CH_3OCH_2]^+$ Revisited: Experimental and Theoretical Study 176
H. E. AUDIER, G. BOUCHOUX, T. B. McMAHON, A. MILLIET AND T. VULPIUS

A New Window on Fullerene Chemistry: An Electrospray Mass Spectrometric Study of the Amination of C_{60} 186
S. R. WILSON AND Y. WU

Significant Differences in Site of Protonation and Extent of Fragmentations in Chemical Ionization and Fast Atom Bombardment Mass Spectrometry of Simple Bifunctional Compounds. A Mechanistic Implication for Formation of Protonated Molecules 192
H. NAKATA, N. ARAKAWA AND R. MIZUNO

Fast Atom Bombardment Mass Spectrometric Study of Benzyloxycarbonyl-protected Tetrapeptides Containing Proline 197
H. TSUNEMATSU, H. HANAZONO, K. HORIE, T. FUKUDA AND M. YAMAMOTO

Negative-ion Fast Atom Bombardment Mass Spectrometry of *N*-Phosphoamino Acids 201
Y.-W. YIN, Y. MA, Y.-F. ZHAO, B. XIN AND G.-H. WANG

OMS Letters
Unexpected Isotope Exchange Reaction of Oxazolidines Under Ammonia Chemical Ionization 205
P.-L. LEHTELÄ AND P. VAINIOTALO

Matrix-assisted Laser Desorption: Dependence of the Threshold Fluence on Analyte Concentration 207
N. MEDINA, T. HUTH-FEHRE, A. WESTMAN AND B. U. R. SUNDQVIST

Book Review 210; Diary 211; Conference Announcement 212

NUMBER 5 MAY 1994

The Efficiency of Collision-induced Ionization of Fast Neutrals: Effects of Neutral Internal Energy and Neutral Translational Energy 213
D. HARNISH AND J. L. HOLMES

Evaluation of Fast Atom Bombardment Mass Spectrometric and Low-energy Collisional Activation Tandem Mass Spectrometric Data for the Structural Elucidation of Bisbenzylisoquinoline Alkaloids 220
G. W. CALDWELL, J. A. MASUCCI AND W.-N. WU

Gas-phase Studies on Reductive Cyclization to a Benzotriazole Derivative from its Precursors by Liquid Chromatography/Thermabeam Tandem Mass Spectrometry 226
D. KUILA AND S. HUANG

Study of Two Diastereomeric Pairs of Regiosomeric 2-Isoxazolines by Tandem Mass Spectrometry with Electron Impact Ionisation 232
A. SELVA, S. AURICCHIO AND A. M. TRUSCELLO

Li^+- and Ag^+-Cationized Per-*O*-acetyl- and Per-*O*-benzyl-α-D-thioglycosides: a Collision-induced Decomposition Study 238
K. P. MADHUSUDANAN, T. S. DHAMI, S. KATIYAR AND S. N. SURYAWANSHI

Fast Atom Bombardment Mass Spectrometric Study of Some Unsaturated Aryl *C*-Glycosides 247
D. SINOU, M. BECCHI AND G. D. DAVES JR

Utility of Nicotinoyl Derivatives in Structural Studies of Mono- and Diacylglycerols by Gas Chromatography/Mass Spectrometry (Part 1) 253
P. ZÖLLNER, E. LORBEER AND G. REMBERG

Differentiation Among the Four Diastereomers of Benzyloxycarbonyl-protected γ-Hydroxyornithine in Negative-ion Fast Atom Bombardment Mass Spectrometry 260
H. TSUNEMATSU, R. ISOBE, K. MIZUSAKI, S. MAKISUMI AND M. YAMAMOTO

Simple Determination of Relative Hydrogen Atom Affinities by Supercritical Fluid Chromatography/Atmospheric Pressure Chemical Ionization Mass Spectrometry 266
K. MATSUMOTO

OMS Letter
Relationship Between Mass Displacements and Dipole Moments of *para*-Substituted Pyridine Odd-electron Molecular Ions 269
O. BORTOLINI, G. SPALLUTO AND P. TRALDI

NUMBER 6 JUNE 1994

Evaluation of the Dipole Moments of Organic Ions in Gas Phase 273
O. BORTOLINI, L. OLIMPIERI AND P. TRALDI

Field-dependent $[M-2H]^{+\cdot}$ Formation in the Field Desorption Mass Spectrometric Analysis of Hydrocarbon Samples 277
C. E. HEINE AND M. M. GEDDES

Structural and Substituent Effects on $[M]^{+\cdot}$ *vs.* $[MH]^+$ Formation in Fast Atom Bombardment Mass Spectra of Simple Organic Compounds 283
H. NAKATA AND K. TANAKA

Multiply Charged Ions of Ruthenium(II), Rhodium(III) and Cobalt(III) Complexes in Electrospray Ionization Mass Spectrometry 289
R. ARAKAWA, T. MATSUO, H. ITO, I. KATAKUSE, K. NOZAKI, T. OHNO AND M.-A. HAGA

Chemical Ionization Mass Spectra of Simple 1,3-Dioxolanes and Their Sulphur Analogues Recorded with Methane, Isobutane, Ammonia and Acetone as Reagent Gas 295
A. LEINONEN AND P. VAINIOTALO

Electron Impact-induced Fragmentation of 2,3-Dihydro-1,5-benzothiazepine-4-(5*H*)-ones 303
G. PÓCSFALVI, A. LÉVAI, Z. DINYA, Á. SOMOGYI AND K. VÉKEY

Mass Spectral Characterization of 3,4,6-Tri-*O*-benzyl-β-*C*-glucopyranosides Containing XC_6H_4S Substituents at C(2) 309
B. V. ROZYNOV, R. J. LIUKKONEN, R. M. CARLSON, D. W. KUEHL, I. P. SMOLIAKOVA, R. CAPLE, C. J. KUEHL AND W. A. SMIT

Dimethyl Ether and Dimethyl d_6 Ether Chemical Ionization Mass Spectrometry of Nitramines, Nitroaromatics and Related Compounds 315
E. P. BURROWS

Differentiation and Electron Ionization-induced Isomerization of 4,5-Bis(alkylthio)-1,3-dithiole-2-thiones and 1,2-Dithiole-3-thiones 321
R. ANDREU, I. GAYÁN, J. GARIN, J. ORDUNA AND M. SAVIRÓN

Metastable Ion Studies: Ethyl(methoxy)(chloro)silanes 326
A. P. HAGEN, S. J. HODGE, B. B. RANDOLPH AND J. L. LAING

OMS Letter
Isomerization of Ionized Toluene and Cycloheptatriene upon Resonant Excitation in a Quadrupole Ion-trap Mass Spectrometer 329
C. BASIC, J. R. EYLER AND R. A. YOST

Diary 333

NUMBER 7 JULY 1994

Electron Impact Ionization Mass Spectra of Lithocholyl Amides: Evidence for a C(20) to C(23) Rearrangement Involving the Loss of a C_4H_9 Fragment 335
P. P. NAIR, V. P. FLANAGAN AND J. E. OLIVER

Mechanism of Stereospecific Alcohol Elimination from Cyclohexane *trans*-1, 3-Dicarboxylates Under Electron Impact Ionization 342
A. ETINGER, A. IDINA AND A. MANDELBAUM

Mass Spectrometry of *N*-Substituted Amino Acids and Their Derivatives: Correlation of the Abundancies of the $M^{+\cdot}$ and the Selected Fragment Ions of Metamers 347
E. WYRZYKIEWICZ AND D. PRUKALA

A Linear Free Energy Correlation in the Low-energy Tandem Mass Spectra of Protonated Tripeptides Gly-Gly-Xxx 354
D. G. MORGAN AND M. M. BURSEY

Mass Spectra of *n*-Butylboronate Ester Derivatives of the Major Metabolite of Prostaglandin F 360
A. FERRETTI, V. P. FLANAGAN AND J. M. ROMAN

Reactivity of Vinylamine Radical Cation with Neutral Dienes 366
G. BOUCHOUX AND F. PENAUD-BERRUYER

Rapid Screening Technique for Tetrachlorodibenzo-*p*-dioxins in Complex Environmental Matrices by Gas Chromatography/Tandem Mass Spectrometry with an Ion Trap Detector 372
J. B. PLOMLEY, C. J. KOESTER AND R. E. MARCH

Tandem Mass Spectrometry of Peptides: Mechanistic Aspects and Structural Information Based on Neutral Losses. II—Tri- and Larger Peptides 382
M. M. CORDERO AND C. WESDEMIOTIS

OMS Letter
Mass Spectrometric Identification of Polycycloaddition of Arylchlorocarbenes and Fluorenylidene to Buckminsterfullerene 391
M. T. LIU, Y. N. ROMASHIN, M. KUBOTA AND M. OHASHI

NUMBER 8 AUGUST 1994

Isodesmic Reactions and Thermochemistry of Ions 395
V. V. TAKHISTOV AND D. A. PONOMAREV

Letter to the Editor 413
V. V. TAKHISTOV AND D. A. PONOMAREV

Evidence for the Existence of Phosphoazonium (Iminophosphenium) and Arsenoazonium Ions in the Gas Phase by Mass Spectrometry 414
J. M. CURTIS, N. BURFORD AND T. M. PARKS

Disparity Between Solution-phase Equilibria and Charge State Distributions in Positive-ion Electrospray Mass Spectrometry 419
G. WANG AND R. B. COLE

The Reaction of Ionized Propene with Methanol: Comparison to $CH_3OH_2^+$ Formation from Ionized 2-Methylpropanol 428
D. J. MCADOO, G. ZHAO, M. S. AHMED, C. E. HUDSON AND C. S. GIAM

Side-chain Effects on the Fragmentation Behaviour of Alkylthiophenes 432
D. LANGE AND H. BUDZIKIEWICZ

Accurate Mass Measurements of Positive Ions in the Desorption Chemical Ionization Mode 439
S. A. PERGANTIS, C. A. EMOND, L. L. MADILAO AND G. K. EIGENDORF

Structural Analysis of Rapamycin and Related Compounds Using $[M+Li]^+$ Ions Generated by Liquid Secondary Ion Mass Spectrometry 445
J. P. KIPLINGER AND M. A. GUADLIANA

NUMBER 9 SEPTEMBER 1994

Notice to Contributors ii

The Bigglesworth Factor 455
T. MCALLISTER

Direct Identification of Organic Inclusions in Graphite on the Basis of Field Desorption Mass Spectrometry 458
M. V. KOSEVICH, V. A. PASHINSKAYA AND V. S. SHELKOVSKY

Unimolecular Neutral and Ion Kinetics by Variable-time Neutralization–Reionization Mass Spectrometry 463
D. W. KUHNS AND F. TURECEK

From Green Algae to Calcium Inside Buckyballs 470
H. R. ROSE, I. G. DANCE, K. J. FISHER, D. R. SMITH, G. D. WILLETT AND M. A. WILSON

Gas-phase Fragmentation Reactions of Protonated Glycerol and its Oligomers: Metastable and Collision-Induced Dissociation Reactions, Associated Deuterium Isotope Effects, and the Structures of $[C_3H_5O]^+$,$[C_2H_5O]^+$,$[C_2H_4O]^{+\cdot}$, and $[C_2H_3O]^+$ Ions 475
C. DASS

Collision Gas Effects in the Collision-Induced Decomposition of Protonated and Cationized Molecules of Carbohydrate Antibiotics 483
M. H. FLORENCIO, D. DESPEYROUX AND K. R. JENNINGS

Fragmentation of Collisionally Activated Hydroxyphenoxide Anions in the Gas Phase 491
R. W. BINKLEY, G. W. DILLOW, T. W. FLECHTNER, W. WINNIK AND M. J. S. TEVESZ

Differentiation of Diastereomeric Chlorin Derivatives by Fast Atom Bombardment Mass Spectrometry 496
P. SCHULZE, D. KUSCH, A. MEIER AND F.-P. MONTFORTS

Novel Use of an Isotope Separator to Determine the Position of Fluorin-18 in Labelled 1,1,1,2-Tetrafluororethanes 499
V. W. PIKE, S. L. WATERS, F. I. AIGBIRHIO, J. MAKEPEACE AND R. J. TANNER

Collisional-activated Decomposition of Benzyloxycarbonyl-protected Tripeptide Derivatives Containing Proline in Fast Atom Bombardment Mass Spectrometry 505
H. TSUNEMATSU, M. YAMAMOTO AND R. ISOBE

C_{60}-assisted Laser Desorption-Ionization Mass Spectrometry 512
L. MICHALAK, K. J. FISHER, D. S. ALDERDICE, D. R. JARDINE AND G. D. WILLETT

NUMBER 10 OCTOBER 1994

Characterization of Explosives by Liquid Chromatography/Mass Spectrometry and Liquid Chromatography/Tandem Mass Spectrometry Using Electrospray Ionization and Parent-Ion Scanning Techniques 517
B. CASETTA AND F. GAROFOLO

Electrospray *vs.* Matrix-assisted Laser Desorption/Ionization. 1. Some Examples in the Protein Field 526
D. FAVRETTO, R. SERAGLIA, P. TRALDI, O. CURCURUTO AND M. HAMDAN

A Mass Spectrometric Investigation on Some 3-[2-(Nitroxy)alkyl]-2*H*-1,3-benzoxazin-4-(3*H*)-one Derivatives 533
E. RIZZI, F. FERRARIO, A. SALA, D. FAVRETTO, S. CATINELLA AND P. TRALDI

On the Gas-phase Reaction of $C_3O_2^{+\cdot}$ with C_3O_2 540
L. PANDOLFO, G. PAIARO, À. SOMOGYI, S. CATINELLA AND P. TRALDI

Investigation of Several Aminoglycoside Solutions Containing One or More Components by Positive Electrospray Mass Spectrometry 547
O. CURCURUTO, G. KENNEDY AND M. HAMDAN

Negative-Ion Fast Atom Bombardment Mass Spectrometry in the Characterization of Deoxyfluorinated Sugars 553
M. COPPOLA, D. FAVRETTO, P. TRALDI AND G. RESNATI

The Potential of Pyrolysis/Gas Chromatography/Mass Spectrometry for Determining the Progress of Lignification: an Investigation of Maturing Asparagus Sclerenchyma Tissue 556
F. A. MELLON, K. W. WALDRON, R. R. SELVENDRAN AND G. C. GALLETTI

Curie-point Pyrolysis Gas Chromatography/Mass Spectrometry in the Identification of Paint Media 561
M. CARBINI, S. VOLPIN AND P. TRALDI

Fast Atom Bombardment Mass Spectrometry of New Polydentate Shiff Bases. 2. The Case of Mono- and Bisaldimines Containing Pyridine Groups 566
M. COPPOLA, S. CATINELLA, P. TRALDI, P. GUERRIERO, S. TAMBURINI AND P. A. VIGATO

Proximity Effects in Mass Spectrometry. Electron Ionization-induced Cyclization of 1,2-Bis(1,4-dithiafulven-6-yl)benzenes 571
P. FRÈRE, A. GORGUES, J. GARÍN AND J. ORDUNA

Gas Chromatographic/Mass Spectrometric Determination of Vinyl Acetate Levels in Air 575
A. STURARO, G. PARVOLI, L. DORETTI, C. BANCOMINA AND C. NEONATO

NUMBER 11 NOVEMBER 1994

Heats of Formation of Multi-substituted Positive Ions of Organic Species 579
Y.-R. LUO, Y. AN AND J. L. HOLMES

Electrospray Mass Spectra of Protein Cations formed in Basic Solutions 587
J. C. Y. LE BLANC, J. WANG, R. GUEVREMONT AND K. W. M. SIU

A Tandem Mass Spectrometric Study of $C_2H_5I^+CH_3$ Ions: a Search for the Non-classical Ethyl Cation Stabilized by Methyl Iodide 594
D. V. ZAGOREVSKII AND J. L. HOLMES

Formation of $M^{+\cdot}$ Ions Under Matrix Fast Atom Bombardment Conditions: Does Charge Exchange Reaction Occur? 601
M. TAKAYAMA, M. IWAMURA AND S. FUCHIBE

Pyrolysis/Gas Chromatography/Mass Spectrometry of Asphaltene Fractions 607
M. NALI, V. CALEMMA AND L. MONTANARI

Translational Energy Losses of LiF Cluster Ions 615
K. VÉKEY AND K. LUDÁNYI

Fast Atom Bombardment Mass Spectrometry of Reaction Products Between C_3O_2 and Stabilized Phosphorus Ylides 619
R. SERAGLIA, P. TRALDI, R. BERTANI, G. FACCHIN AND L. PANDOLFO

Mass Spectral Fragmentation Pathways in Some Glycoluril-type Explosives. A Study by Collision-induced Dissociation and Isotope Labeling 625
J. YINON, S. BULUSU, T. AXENROD AND H. YAZDEKHASTI

Investigation of Cationic Organic Dyes Used as Molecular Probes by Liquid Secondary Ion Mass Spectrometry 632
R. E. CARLSON AND K. L. BUSCH

Resonance Electron Capture for Determining Double Bound and Hydroxy Group Location in Fatty Acids 641
V. G. VOINOV, V. M. BOGUSLAVSKIY AND Y. N. ELKIN

Mass Spectrometric Behaviour of Simple Oxazolidines Under Electron Impact and Chemical Ionization 647
P.-L. LEHTELÄ, R. SMOLANDER AND P. VAINIOTALO

Characterization of Modification Sites During Peptide Synthesis Using Liquid Secondary Ion/Collision-induced Dissociation Mass Spectrometry and a Computer Program 654
J. ROZENSKI, I. SAMSON, G. JANSSEN, R. BUSSON, A. VAN AERSCHOT AND P. HERDEWIJN

Multiphonon Ionization and Photodissociation at Second-order Space Focus in a Time-of-flight Mass Spectrometer: the Amino Acid Tryptophan 659
M. DEY AND J. GROTEMEYER

Determination of Tetrahydrocannabinolic Acid–Carrier Protein Conjugate by Matrix-assisted Laser Desorption/Ionization Mass Spectrometry and Antibody Formation 668
Y. GOTO, Y. SHIMA, S. MORIMOTO, Y. SHOYAMA, H. MURAKAMI, A. KUSAI AND K. NOJIMA

Characterization of Chlorins within a Natural Chlorin Mixture Using Electrospray/Ion Trap Mass Spectrometry 672
X. Fr. D. CHILLIER, G. J. VAN BERKEL, F. O. GÜLAÇAR AND A. BUCHS

Fragment Ion Formation From *n*-Alkanes and Cycloalkanes by Plasma Desorption 679
R. L. BETTS, M. A. PARK, E. L. SHIREY AND E. A. SCHWEIKERT

OMS Letters
Electron Impact Mass Spectrometry of Some Potential Neuroleptic *trans*-(2-Amino Methyl)-Cycloalkyl Aryl Ketones 685
J. M. BLANCO, O. CAAMANO, E. URIARTE, G. DELOGU, G. PODDA, R. SERAGLIA AND P. TRALDI

Perfluorokerosene, Fomblin M and Ultramark 1621 as Mass Calibrants in Tandem Mass Spectrometry 690
J. H. LAMB, G. M. A. SWEETMAN AND S. NAYLOR

Simultaneous Trapping of Positive and Negative Ions Using a Nested Open-ended Trapped-ion Cell in Fourier Transform Ion Cyclotron Resonance Mass Spectrometry 692
V. H. VARTANIAN AND D. A. LAUDE

Identification by Tandem-Mass Spectrometry of the Very Rare β-Carotenone Isolated from the Leaves of Two Cycads 695
A. SELVA, F. CARDINI AND M. CHELLI

Fragmentation of *O*-Isopropylidene Derivatives of 1,2-Diols on Electron Impact 698
J.-F. RONTANI AND C. AUBERT

Linkage Position Determination of Lithium-cationized Disaccharides by Surface-induced Dissociation Tandem Mass Spectrometry 700
A. R. DONGRÉ AND V. H. WYSOCKI

NUMBER 12 DECEMBER 1994

Editorial 705

Fast Atom Bombardment Mass and Tandem Mass Spectra of Protonated and Alkali Cationized Aldobiouronic and Pseudoaldobiouronic Acid Per-*O*-methyl Derivatives 707
V. KOVÁČIK, J. HIRSCH, W. HEERMA, C. G. De KOSTER AND J. HAVERKAMP

Tandem Mass Spectrometric Analysis of Fixed-charge Derivatized Oligosaccharides 713
B. DOMON, D. R. MUELLER AND W. J. RICHTER

Liquid Secondary Ionization, Tandem and Matrix-assisted Laser Desorption/Ionization Time-of-flight Spectrometric Characterization of Glycosphingolipid Derivatives 720
H. PERREAULT AND C. E. COSTELLO

Profiling Glycosphingolipid Structural Detail: Periodate Oxidation, Electrospray, Collision-induced Dissociation, and Tandem Mass Spectrometry 736
B. B. REINHOLD, S.-Y. CHAN, S. CHAN AND V. N. REINHOLD

Potentials of Electrospray Mass Spectrometry for Structural Studies of *O*-Glycoamino Acids and -Peptides with Multiple α2,6-Sialosyl-Tn Glycosylation 747
J. PETER-KATALINIĆ, A. ASHCROFT, B. GREEN, F.-G. HANISCH, Y. NAKAHARA, H. ILIJIMA AND T. OGAWA

Examination of Complex Oligosaccharides by Matrix-assisted Laser Desorption Mass Spectrometry on Time-of-flight and Magnetic Sector Instruments 753
D. J. HARVEY, P. M. RUDD, R. H. BATEMAN, R. S. BORDOLI, K. HOWES, J. B. HOYES AND R. G. VICKERS

Structure Determination of Phosphoinositol Oligosaccharides from Parasitic Protozoa Using Fast Atom Bombardment Mass Spectrometry 767
R. WAIT, C. JONES, F. H. ROUTIER, J. O. PREVIATO AND L. MENDONÇA-PREVIATO

Structure Analysis of Branched Oligosaccharides Using Post-source Decay in Matrix-assisted Laser Desorption Ionization Mass Spectrometry 782
B. SPENGLER, D. KIRSCH, R. KAUFMANN AND J. LEMOINE

Reactions of Ionized Dibutyl Ether 791
R. D. BOWEN, D. SUH AND J. K. TERLOUW

Characterisation of Organoboron Ligands by Electrospray Mass Spectrometry Using Anhydrous Solvent Application 806
F. LIBOT, H. VIRELIZIER, O. FROELICH, M. BONIN, J.-C. QUIRION AND H.-P. HUSSON

Isomerization of Phytyl Ethers on Electron Impact 808
J.-F. RONTANI